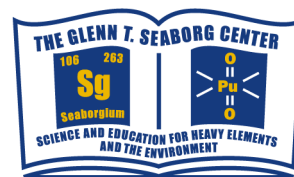




Glenn T. Seaborg Center Seminar



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Activating Fluoroalkanes and Fluoroarenes with Lanthanocenes Hydride Complexes

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4 pm

Building 70A-3377

Abstract

Metal complexes are known to activate inert bonds. While considerable success has been met in the case of H-H and C-H bonds, fewer complexes have been found to activate a C-F bond. This is often attributed to the strength of the C-F bond; however, this does not rationalize the experimental fact because even stronger M-F bonds are often formed during the chemical transformation. Computational studies on selected cases reveal that there is often no thermodynamic disadvantage in cleaving a C-F bond but that substantial kinetic barriers may be present. In the case of lanthanocene-hydride complexes, the very strong affinity of the lanthanide center for fluoride allows defluorination of hydrofluoromethanes and hydrofluorobenzenes to occur (R.A. Andersen). DFT calculations offer mechanistic help in understanding these transformations.